Quantum scattering in one dimension

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Abstract

A self-contained discussion of nonrelativistic quantum scattering is presented in the case of central potentials in one space dimension, which will facilitate the understanding of the more complex scattering theory in two and three dimensions. The present discussion illustrates in a simple way the concept of partial-wave decomposition, phase shift, optical theorem and effective-range expansion.

I. INTRODUCTION

There has been great interest in studying tunneling phenomena in a finite superlattice [1], which essentially deals with quantum scattering in one dimension. It has also been emphasized [2] that a study of quantum scattering in one dimension is important for the study of Levinson's theorem and virial coefficient. Moreover, one-dimensional quantum scattering continues as an active line of research [3]. Because of these recent interests we present a comprehensive description of quantum scattering in one dimension in close analogy with the two- [4] and three-dimensional cases [5]. Apart from these interests in research, the study of one-dimensional scattering is also interesting from a pedagogical point of view. In a one dimensional treatment one does not need special mathematical functions, such as the Bessel's functions, while still retaining sufficient complexity to illustrate many of the physical processes which occur in two and three dimensions. Hence the present discussion of one dimensional scattering is expected to assist the understanding of the more complex two and three dimensional scattering problems.

A self-contained discussion of two-dimensional scattering has appeared in the literature [4]. It is realized that the scattering amplitude which arises from the usual asymptotic form of the scattering wave function in three dimensions is not the most satisfactory one in two dimensions and a modified scattering amplitude has been proposed in this case. However, this modification in the case of two dimensions can not be extended to one-dimensional scattering in a straightforward way, basically because in one dimension there are only two discrete scattering directions: forward and backward along a line. This requires special techniques in one dimension in distinction with two or three dimension where an infinity of scattering directions are permitted characterized by continuous angular variable(s).

It is because of the above subtlety of the one-dimensional scattering problem we present a complete discussion of this case. Here we present a new relation between the asymptotic wave function and the scattering amplitude with desirable analytic properties and consequently, present a discussion of one-dimensional scattering which should be considered complimentary to the discussion of two-dimensional scattering of Ref. [4].

In Sec. 2 we present a wave-function description of scattering with a convenient partial wave analysis. Section 3 illustrates the the formulation of effective-range expansion. A brief summary is presented in Sec. 4.

II. WAVE-FUNCTION DESCRIPTION

In one dimension the scattering wave function $\psi_k^{(+)}(x)$ at position x satisfies the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \right] \psi_k^{(+)}(x) = E\psi_k^{(+)}(x) \tag{1}$$

where $V(x)$ is a centrally-symmetric finite-range potential satisfying $V(x) = 0, x_0 \equiv |x| > R$ and $V(x) = V(-x)$, where m is the reduced mass, $E \equiv \hbar^2 k^2/(2m)$ the energy and k the wave number.

The asymptotic form of the wave function is taken as

$$\lim_{x_0 \to \infty} \psi_k^{(+)}(x) \to \exp(ikx) + \frac{i}{k} f_k^{(+)}(\epsilon) \exp(ikx_0) \tag{2}$$

where $\epsilon = x/x_0$, $f_k^{(+)}(\epsilon)$ is the scattering amplitude, $\exp(ikx)$ the incident plane wave and $\exp(ikx_0)$ the scattered outgoing wave. There are two discrete directions in one dimension characterized by signs of x and given by $\epsilon = \pm 1$ in contrast to infinite possibility of scattering angles in two and three dimensions. The forward (backward) direction is given by the positive (negative) sign. The discrete differential cross sections in these two directions are given by

$$\sigma_\epsilon = \frac{1}{k^2} |f_k^{(+)}(\epsilon)|^2 \tag{3}$$

and the total cross section by

$$\sigma_{\text{tot}} = \sum_\epsilon \sigma_\epsilon = \frac{1}{k^2} \left[|f_k^{(+)}(+)|^2 + |f_k^{(+)}(-)|^2 \right]. \tag{4}$$

The discrete sum in (4) is to be compared with integrals over continuous angle variables in two and three dimensions. The two differential cross sections (3) are the usual reflection and transmission probabilities. An extra factor of i is introduced in the outgoing wave part of (2). This will have the advantage of leading to an optical theorem in close analogy with the three-dimensional case [5] as we shall see in the following.

In order to define the partial-wave projection of the wave function and partial-wave phase shifts, we consider the following parametrization of the asymptotic wave function

$$\lim_{x_0 \to \infty} \psi_k^{(+)}(x) = \sum_{L=0}^{1} \epsilon^L A_L \cos \left[kx_0 + \frac{L\pi}{2} + \delta_L(k^2) \right] \tag{5}$$

where δ_L is the scattering phase shift for the Lth wave and A_L is an unknown coefficient. In contrast to the infinite number of partial waves in two and three dimensions, two partial waves are sufficient in this case. Also, one has the following partial-wave projection for the incident wave

$$\exp(ikx) = \cos(kx_0) + i\epsilon \sin(kx_0). \tag{6}$$

Consistency between (2) and (5) yields $A_L = (-i)^L \exp(i\delta_L)$ and

$$f_k^{(+)}(\epsilon) = k \sum_{L=0}^{1} \epsilon^L \exp(i\delta_L) \sin(\delta_L). \tag{7}$$

Now one naturally defines the partial-wave amplitudes

$$f_L = k \exp(i\delta_L) \sin(\delta_L) \tag{8}$$

in terms of phase shift δ_L so that the total cross section of (4) becomes

$$\sigma_{\text{tot}} = 2 \sum_{L=0}^{1} \sin^2(\delta_L) \tag{9}$$

and satisfies the following optical theorem

$$\sigma_{\text{tot}} = \frac{2}{k}\Im f_k^{(+)}(+),\tag{10}$$

in close analogy with the three-dimensional case, where $\Im$ is the imaginary part. Had we not introduced i in the asymptotic form (2), this optical theorem would involve the real part of the forward scattering amplitude in place of the imaginary part. This factor of i has no consequence on the observables.

In partial waves $L = 0, 1$, the Schrödinger equation (1) becomes

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx_0^2} + V(x_0) \right] \psi_{k,L}^{(+)}(x_0) = E\psi_{k,L}^{(+)}(x_0)\tag{11}$$

where $x_0 \equiv |x|$ by definition is positive. The two solutions − symmetric and antisymmetric, corresponding to $L = 0$ and 1, respectively − are constructed from (11) using the asymptotic condition (5).

III. EFFECTIVE-RANGE EXPANSION

Next we illustrate the formulation of the last section by developing an effective-range expansion in both partial waves $L = 0$ and 1 in close analogy with three dimensions. There are some specific difficulties in the two dimensional case which we shall not consider here [6]. In both partial waves the radial Schrödinger equation can be written as

$$\left[\frac{d^2}{dx_0^2} + k^2 - U(x_0) \right] \psi_{k,L}^{(+)}(x_0) = 0,\tag{12}$$

where $U(x_0) = 2mV(x_0)/\hbar^2$. The $L = 0$ wave involves the symmetric solution and the $L = 1$ wave the antisymmetric solution. The solution of (12) behaves like $\psi(x_0) = \chi(kx_0)$ near $x_0 = 0$ and $\psi(x_0) = \chi[kx_0 + \delta_L(k^2)]$ in the asymptotic region, $x_0 \to \infty$. The function χ is a sine function for $L = 1$ and a cosine one for $L = 0$. This compact notation will simplify the treatment of the effective-range expansion. The treatment of the $L = 1$ solution in one dimension is essentially identical with that of the S-wave potential scattering in three dimensions. The similarity between the present one-dimensional treatment for $L = 1$ and the S-wave potential scattering in three dimensions suggests that the usual form of Levinson's theorem in three dimensions will be valid in this case, e.g., $\delta_1(0) - \delta_1(\infty) = n\pi$, where n is the number of $L = 1$ bound states in one dimension [2].

We consider two solutions u_1 and u_2 at two energies k_1^2 and k_2^2 of the Schrödinger equation (12). These solutions are normalized such that asymptotically

$$\lim_{x_0 \to \infty} u_i(x_0) \to \frac{\chi[k_i x_0 + \delta_L(k_i^2)]}{\chi[\delta_L(k_i^2)]}\tag{13}$$

where $i = 1$ and 2 refer to the two energies k_1^2 and k_2^2, respectively. From the two equations (12) satisfied by the functions u_1 and u_2 we readily obtain as in the three-dimensional case

$$[u_2(x_0)u_1'(x_0) - u_1(x_0)u_2'(x_0)]_0^R = (k_2^2 - k_1^2) \int_0^R u_1(x_0)u_2(x_0)dx_0 \tag{14}$$

where R is an arbitrary radial distance and the prime on the function u denotes derivative with respect to x_0.

Next we consider two free-particle solutions

$$v_i(x_0) = \frac{\chi[k_i x_0 + \delta_L(k_i^2)]}{\chi[\delta_L(k_i^2)]} \tag{15}$$

of (12) obtained by putting $U(x_0) = 0$. Then we have

$$[v_2(x_0)v_1'(x_0) - v_1(x_0)v_2'(x_0)]_0^R = (k_2^2 - k_1^2) \int_0^R v_1(x_0)v_2(x_0)dx_0. \tag{16}$$

With these general equations first we specialize to the case of $L = 1$. Subtracting (16) from (14), using (13) and (15) and the conditions $u_1(0) = u_2(0) = 0$ and letting R go to ∞, one gets

$$k_2 \cot \delta_1(k_2^2) = k_1 \cot \delta_1(k_1^2) + (k_2^2 - k_1^2) \int_0^\infty [v_1(x_0)v_2(x_0) - u_1(x_0)u_2(x_0)]dx_0. \tag{17}$$

It is convenient to define the $L = 1$ scattering length a_1 in analogy with three dimensions by

$$-\frac{1}{a_1} = \lim_{k \to 0} k \cot \delta_1(k^2). \tag{18}$$

Now letting $k_1 = 0$ and denoting $k_2 = k$ in (17) we have

$$k \cot \delta_1(k^2) = -\frac{1}{a_1} + k^2 \int_0^\infty [v_0(x_0)v_k(x_0) - u_0(x_0)u_k(x_0)]dx_0 \tag{19}$$

where the suffix 0 or k on the wave function refers to the energy. Next making a power-series expansion of the integral in (19), we get the one-dimensional effective-range expansion

$$k \cot \delta_1(k^2) = -\frac{1}{a_1} + \frac{1}{2}r_1 k^2 + O(k^4) + ... \tag{20}$$

with

$$r_1 = 2 \int_0^\infty [v_0^2(x_0) - u_0^2(x_0)]dx_0 \tag{21}$$

where u_0 and v_0 are the zero-energy solutions and r_1 the effective range for $L = 1$.

The meaning of scattering length and effective range becomes more explicit if we consider the symmetric one-dimensional square well defined by $U(x_0) = 0$ for $x_0 > R$ and $U(x_0) = -\beta_0^2$ for $x_0 < R$. The solution of the Schrödinger equation in this (antisymmetric) case is given by

$$u(x_0) = B_1 \sin(\beta x_0), \quad x_0 < R \tag{22}$$
$$= A_1 \sin[kx_0 + \delta_1(k^2)], \quad x_0 > R \tag{23}$$

where $\beta^2 = k^2 + \beta_0^2$. By matching the log derivative at $x_0 = R$ one gets $k \cot[kR + \delta_1(k^2)] = \beta \cot(\beta R)$. This condition can be rewritten as

$$k \cot \delta_1(k^2) = \frac{k^2 \tan(\beta R) \tan(kR) + k\beta}{k \tan(\beta R) - \beta \tan(kR)}. \tag{24}$$

A straightforward low-energy expansion of (24) and comparison with (20) yield

$$a_1 = R - \frac{1}{\beta_0} \tan(\beta_0 R) \tag{25}$$

$$r_1 = 2R - 2\frac{R^2}{a_1} + \frac{2R^3}{3a_1^2} + \left(1 - \frac{R}{a_1}\right)^2 \left(\frac{1}{\beta_0 \tan(\beta_0 R)} - \frac{R}{\sin^2(\beta_0 R)}\right). \tag{26}$$

In this case the first bound state appears for $\beta_0 R > \pi/2$ and a new bound state appears as $\beta_0 R$ crosses $(2n+1)\pi/2$ where n is a positive integer including 0. So the system will have n bound states for $(2n-1)\pi/2 < \beta_0 R < (2n+1)\pi/2$. The scattering length a_1 tends to infinity as $\beta_0 R \to (2n+1)\pi/2$, which denotes the appearance of a new bound state. Also, as a new bound state appears, $a_1 \to \infty$ and r_1 of (26) tends to R the range of square well. This is why the name effective range is given to r_1.

Next we consider the case of $L = 0$. Although the $L = 1$ case discussed above is quite similar to the three dimensional case for $L = 0$, the $L = 0$ case described below has no three-dimensional analogue. Nevertheless we describe this case for the sake of completeness. Subtracting (16) from (14), using (13) and (15) and the conditions $u_1'(0) = u_2'(0) = 0$ and letting R go to ∞, one gets

$$k_2 \tan \delta_0(k_2^2) = k_1 \tan \delta_0(k_1^2) - (k_2^2 - k_1^2) \int_0^\infty [v_1(x_0)v_2(x_0) - u_1(x_0)u_2(x_0)]dx_0. \tag{27}$$

It is convenient to define the $L = 0$ scattering length a_0 by

$$\frac{1}{a_0} = \lim_{k \to 0} k \tan \delta_0(k^2). \tag{28}$$

Now letting $k_1 = 0$ and denoting $k_2 = k$ in (27) we have

$$k \tan \delta_0(k^2) = \frac{1}{a_0} - k^2 \int_0^\infty [v_0(x_0)v_k(x_0) - u_0(x_0)u_k(x_0)]dx_0 \tag{29}$$

where the suffix 0 or k on the wave function refers to the energy. A power-series expansion of (29) in energy leads to

$$k \tan \delta_0(k^2) = \frac{1}{a_0} + \frac{1}{2}r_0 k^2 + O(k^4) + \dots \tag{30}$$

where the effective range is given by

$$r_0 = -2 \int_0^\infty [v_0^2(x_0) - u_0^2(x_0)]dx_0. \tag{31}$$

The solution of the Schrödinger equation in this case for the one-dimensional square well defined by $U(x_0) = 0$ for $x_0 > R$ and $U(x_0) = -\beta_0^2$ for $x_0 < R$ is given by

$$u(x_0) = B_0 \cos(\beta x_0), \quad x_0 < R \tag{32}$$
$$= A_0 \cos[kx_0 + \delta_0(k^2)], \quad x_0 > R \tag{33}$$

By matching the log derivative at $x_0 = R$ one gets $k \tan[kR + \delta_0(k^2)] = \beta \tan(\beta R)$. This condition can be rewritten as

$$k \tan \delta_0(k^2) = \frac{k\beta \tan(\beta R) - k^2 \tan(kR)}{k + \beta \tan(\beta R) \tan(kR)}. \tag{34}$$

A straightforward low-energy expansion of (34) and comparison with (30) yield

$$a_0 = R + \frac{1}{\beta_0 \tan(\beta_0 R)} \tag{35}$$

$$r_0 = 2R - 2\frac{R^2}{a_0} + \frac{2R^3}{3a_0^2} - \left(1 - \frac{R}{a_0}\right)^2 \left(\frac{\tan(\beta_0 R)}{\beta_0} + \frac{R}{\cos^2(\beta_0 R)}\right) \tag{36}$$

In this case there is at least one bound state for all values of $\beta_0 R$ and a new bound state appears as $\beta_0 R$ crosses $n\pi$ where n is a positive integer including 0. So the system will have n bound states for $(n-1)\pi < \beta_0 R < n\pi$. The scattering length a_0 tends to infinity as $\beta_0 R \to n\pi$ denoting the appearance of a new bound state. Also, as a new bound state appears, $a_0 \to \infty$, and r_0 of (36) tends to R the range of square well. This is why the name effective range is given to r_0 in this case.

IV. SUMMARY

In this paper we have generalized the standard treatments of two- and three-dimensional scattering to the case of one-dimensional scattering. We have introduced the concept of scattering amplitude, partial wave, phase shift, optical theorem and effective-range expansion in close analogy with three-dimensional scattering. In this case there are two partial waves: $L = 0$ and 1. The quantum mechanical one-dimensional scattering is mathematically a much simpler problem compared to that in two and three dimensions. The present discussion of one-dimensional scattering deviod of the usual mathematical complexity encountered in two and three dimensions will help one to understand easily the different physical concepts of general scattering theory.

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